Intro To Perturbation Theory *

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I.

Assuming a soluble Hamiltonian H_0 and a "true" Hamiltonian H_{true} such that the difference between the two can be considered in some sense "small", one has

$$H_{true}\Psi = E\Psi$$

as the equation we wish to solve. Let's write the true Hamiltonian as

$$H_0 + \lambda H'$$

so that we can change λ from zero (no perturbation) to one, where the perturbation is fully effective. We have, if H_0 was well chosen

$$H_0\Psi_i^0 = E_i^0\Psi_i^0$$

where i is the quantum number of the state with the appropriate energy and appropriate wave (eigen) function.

We wish to solve the equation

$$\left(H_0 + \lambda H'\right)\Psi_n = E_n\Psi_n$$

and, for the time being, we assume that all wave functions under discussion are non-degenerate!

We expand the wave function and eignenergy of the true problem in powers of λ and collect terms of similar powers of λ together. We have

$$\Psi_n = \Psi_n^0 + \lambda\Psi_n^{(1)} + \lambda^2\Psi_n^{(2)} + \cdots \tag{1}$$

and

$$E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \tag{2}$$

Of course, we assume that each added order of correction is smaller than its predecessors. We then have

$$\begin{aligned}\left(H_0 + \lambda H'\right)\Psi_n^0 + \lambda\Psi_n^{(1)} + \lambda^2\Psi_n^{(2)} + \cdots = \\ \left(E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\right) \\ \left(\Psi_n^0 + \lambda\Psi_n^{(1)} + \lambda^2\Psi_n^{(2)} + \cdots\right)\end{aligned} \tag{3}$$

i.e.,

$$\begin{aligned}H_0\Psi_n^0 + H_0\lambda\Psi_n^{(1)} + H_0\lambda^2\Psi_n^{(2)} + \cdots\lambda H'\Psi_n^0 + \lambda H'\lambda\Psi_n^{(1)} + \lambda H'\lambda^2\Psi_n^{(2)} + \cdots = \\ E_n^0\Psi_n^0 + E_n^0\lambda\Psi_n^{(1)} + E_n^0\lambda^2\Psi_n^{(2)} + \\ \lambda E_n^{(1)} + \Psi_n^0 + \lambda E_n^{(1)} + \lambda\Psi_n^{(1)} + \lambda E_n^{(1)} + \\ \lambda^2\Psi_n^{(2)} + \lambda^2 E_n^{(2)}\Psi_n^0 + \lambda^2 E_n^{(2)}\lambda\Psi_n^{(1)} + \lambda^2 E_n^{(2)}\lambda^2\Psi_n^{(2)} + \cdots\end{aligned} \tag{4}$$

Obviously, expanding the product and grouping terms by powers of λ leads us to a set of coupled equations:

$$\begin{aligned}H_0\Psi_n^0 = E_n^0\Psi_n^0; \lambda = 0 \\ H_0\Psi_n^{(1)} + H'\Psi_n^{(0)} = E_n^{(0)}\Psi_n^{(1)} + E_n^{(1)}\Psi_n^{(0)}; \lambda = 1 \\ H_0\Psi_n^{(2)} + H'\Psi_n^{(1)} = E_n^{(0)}\Psi_n^{(2)} + E_n^{(1)}\Psi_n^{(1)} + E_n^{(2)}\Psi_n^{(0)}; \lambda = 2 \quad (5) \\ \cdots \quad (6)\end{aligned}$$

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If now, for the first order correction, we use

$$\Psi_n^{(1)} = \sum_i a_{n,i}\Psi_i^{(0)}$$

then the first order equation reads

$$H_0 \sum_i a_{n,i}\Psi_i^{(0)} + H'\Psi_n^{(0)} = E_n^{(0)} \sum_i a_{n,i}\Psi_i^{(0)} + E_n^{(1)}\Psi_n^{(0)};$$

Multiplying by $\Psi_k^{(0)^*}$ and integrating we obtain

$$< k|H^{(1)}|n > + a_{n,k}(E_k^{(0)} - E_n^{(0)}) = E_n^{(1)}\delta_{n,k}$$

II. AN EXAMPLE

Consider a harmonic oscillator with a harmonic perturbation. That means

$$H_{true} = \frac{p^2}{2m} + (k+\lambda)\frac{x^2}{2}$$

where we have added a λ dependent pertubation onto an existing Harmonic Oscillator. Clearly, the exact (true) answer to the complete infinite order pertubation analysis would be energy levels for the $k+\lambda$ force constant H.O.. (see Equation 8)

$$< k|\lambda\frac{x^2}{2}|n > + a_{n,k}(E_k^{(0)} - E_n^{(0)}) = E_n^{(1)}\delta_{n,k}$$

There are two cases we need to deal with, when n=k and when $n \neq k$. For the former we have

$$\frac{\lambda}{2} < n|x^2|n > + zero = E_n^{(0)}$$

which is the correction to the original energy, while for the latter we have

$$a_{n,k} = -\frac{\lambda}{2}\frac{< k|x^2|n >}{E_k^{(0)} - E_n^{(0)}}$$

which is the prescription for obtaining the expansion coöefficients for the first order perturbation wave function.

III. LADDER OPERATOR EVALUATION

We know that $a_+ = p + \imath\hbar\omega x$ and $a_- = p - \imath\hbar\omega x$ so

$$x = \frac{a_+ - a_-}{2\imath\hbar\omega}$$

and therefore

$$x^2 = -\frac{1}{4\hbar^2\omega^2}\left(a_+^2 - a_+a_- - a_-a_+ + a_-^2\right)$$

and since

$$a_-|0 >= (p - \imath m\omega x)|0 >= \imath\hbar\frac{d|0 >}{dx} - \imath m\omega x|0 >= 0$$

one obtains

$$\ell n|0 >= -\frac{m\omega}{\hbar}x^2 + C_1 = \ell n|0 >= C_2 e^{-\frac{m\omega}{\hbar}x^2}$$

where C_2 is a normalization constant.

$$(p + \imath m\omega x)|0> = -\imath\hbar\frac{d|0>}{dx} + \imath m\omega x|0> \rightarrow |1>$$

which means that

$$2\imath m\omega x|0> \rightarrow |1>$$

i.e.,

$$|1> = C_3 x e^{-\frac{m\omega}{\hbar}x^2}$$

$$a+^2|0> \rightarrow |2>$$

and

$$a_- a_+|0> \rightarrow |0>$$

we have

$$< 0|\frac{\lambda x^2}{2}|0> = -\frac{\lambda}{8\hbar^2\omega^2} < 1|1> \tag{7}$$

Remember that there is a question of normalization which has not been addressed, i.e., when laddering up and down, what happens to the normalization?

IV. A MORE DIRECT SCHEME BY BRUTE FORCE INTEGRATION

We know that $E_0^{(0)} = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$ and $E_{true}^{(0)} = \frac{\hbar}{2}\sqrt{\frac{k+\lambda}{m}}$ so, expanding the latter in a Taylor series in λ should result in a power series identical to that obtained by perturbation theory. We have for the ground vibrational state

$$E_{true}^{(0)} = \frac{\hbar}{2}\sqrt{\frac{k+\lambda}{m}} \tag{8}$$

and, expanding

$$E_{true}^{(0)} = \frac{\hbar}{2}\sqrt{\frac{k}{m}} + \left(\frac{\partial E_{true}^{(0)}}{\partial\lambda}\right)_{\lambda=0}\lambda + \cdots$$

$$\left(\frac{\partial E_{true}^{(0)}}{\partial\lambda}\right) = \frac{\hbar}{2}\frac{1}{2}\left(\frac{k+\lambda}{m}\right)^{-1/2}\frac{1}{m} = \frac{\hbar}{4m}\sqrt{\frac{m}{k+\lambda}}$$

$$\left.\left(\frac{\partial E_{true}^{(0)}}{\partial\lambda}\right)\right|_{\lambda=0} = \frac{\hbar}{4m}\left.\sqrt{\frac{m}{k+\lambda}}\right|_{\lambda=0} = \frac{\hbar}{4m}\sqrt{\frac{m}{k}} = \frac{\hbar}{4m\omega}$$

$$E_{true}^{(0)} = \frac{\hbar}{2}\sqrt{\frac{k}{m}} + \frac{\hbar}{4m\omega}\lambda + \cdots \tag{9}$$

Since the ground state wave function is

$$\psi_0(x) = Ce^{-\frac{m\omega}{\hbar}x^2/2}$$

we know that

$$\int_{-\infty}^{\infty} \psi_0(x)^2 dx = 1$$

forces the value of C, i.e.,

$$C = \sqrt{\frac{1}{\int_{-\infty}^{\infty} \left(e^{-\frac{m\omega}{\hbar} x^2/2}\right)^2 dx}} = \sqrt{\frac{1}{\int_{-\infty}^{\infty} \left(e^{-\frac{m\omega}{\hbar} x^2}\right) dx}}$$

meaning that we need to remind ourselves about the integral

$$\int_{-\infty}^{\infty} e^{-\alpha\eta^2} d\eta = \sqrt{\frac{\pi}{\alpha}}$$

yields a value for C

$$C = \sqrt{\frac{1}{\sqrt{\frac{\pi}{\alpha}}}} = C = \sqrt{\frac{1}{\sqrt{\frac{\pi}{\frac{m\omega}{\hbar}}}}} C = \sqrt{\sqrt{\frac{m\omega}{\hbar\pi}}} = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}$$

since $\alpha = \frac{m\omega}{\hbar}$ in our context. Thus

$$\psi_0(x) = \sqrt{\frac{m\omega}{\hbar\sqrt{\pi}}} e^{-\frac{m\omega}{\hbar}\frac{x^2}{2}}$$

we can easily evaluate the term (Equation 7)

We will need the matrix element of x^2, i.e., we will need the integral

$$\int_{-\infty}^{\infty} \eta^2 e^{-\alpha\eta^2} d\eta = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

to ascertain the value of the right hand side of this equation, i.e.,

$$< 0|\frac{\lambda x^2}{2}|0 >= \frac{\lambda}{2}\left(\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\right)^2 \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar} x^2} dx$$

This is a straight forward evaluation, yielding

$$< 0|\frac{\lambda x^2}{2}|0 >= \frac{\lambda}{2}\left(\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}}\right) \frac{1}{2}\sqrt{\frac{\pi}{\left(\frac{m\omega}{\hbar}\right)^3}}$$

or

$$\frac{\lambda}{4}\frac{m^{1/2}\omega^{1/2}}{\hbar^{1/2}}\frac{\hbar^{3/2}}{m^{3/2}\omega^{3/2}}$$

which finally is the desired result, Equation 9,

$$< 0|\frac{\lambda x^2}{2}|0 >= \frac{\lambda}{4}\frac{\hbar}{m\omega}$$